

The linear Fokker-Planck equation for the Ornstein-Uhlenbeck process as an (almost) nonlinear kinetic equation for an isolated N-particle system

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Abstract

It is long known that the Fokker-Planck equation with prescribed constant coefficients of diffusion and linear friction describes the ensemble average of the stochastic evolutions in velocity space of a Brownian test particle immersed in a heat bath of fixed temperature. Apparently, it is not so well known that the same partial differential equation, but now with constant coefficients which are functionals of the solution itself rather than being prescribed, describes the kinetic evolution (in the $N \rightarrow \infty$ limit) of an *isolated* N -particle system with certain stochastic interactions. Here we discuss in detail this recently discovered interpretation.

KEYWORDS: Kinetic theory, Kac program, propagation of chaos, diffusion equation on a high-dimensional sphere, Fokker–Planck equation.

1 Introduction

As is well known, [UhOr30], [Cha43], [Bal75], the ensemble average of the stochastic evolutions in velocity space of a Brownian test particle¹ of unit mass, immersed in a drifting uniform heat bath of fixed temperature T and constant drift velocity \mathbf{u} , is governed by the Fokker–Planck equation with prescribed constant coefficients of diffusion and (linear) friction,

$$\partial_t f(\mathbf{v}; t) = \partial_{\mathbf{v}} \cdot \left(T \partial_{\mathbf{v}} f(\mathbf{v}; t) + (\mathbf{v} - \mathbf{u}) f(\mathbf{v}; t) \right). \quad (1)$$

Here, $f(\cdot; t) : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ is the ensemble’s probability density function on velocity space at time $t \in \mathbb{R}_+$, and an overall constant has been absorbed in the time

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¹For the beginnings of the theory of Brownian motion, see the collection of Einstein’s papers with commentary [Ein85].

scale. Of course, we could also shift \mathbf{v} to obtain $\mathbf{u} = \mathbf{0}$, then rescale \mathbf{v} , t , and f to obtain $T = 1$; however, for pedagogical purposes we refrain from doing so. The solution $f(\mathbf{v}; t)$ of (1) is given by $f(\mathbf{v}; t) = \int_{\mathbb{R}^3} G_t(\mathbf{w}, \mathbf{v}|\mathbf{u}; T) f_0(\mathbf{w}) d^3\mathbf{w}$, where $f_0(\mathbf{v}) \equiv f(\mathbf{v}; 0)$ and

$$G_t(\mathbf{w}, \mathbf{v}|\mathbf{u}; T) = (2\pi T(1 - e^{-2t}))^{-\frac{3}{2}} \exp\left(-\frac{1}{2T} \frac{|\mathbf{v} - \mathbf{u} - \mathbf{w}e^{-t}|^2}{1 - e^{-2t}}\right) \quad (2)$$

is the Green function for (1), see [UhOr30], [Cha43]. In its standard form, i.e. with $T = 1$ and $\mathbf{u} = \mathbf{0}$, (2) is known as the (Mehler) kernel of the adjoint Ornstein-Uhlenbeck semigroup (a.k.a. Fokker-Planck semigroup).

Over the years, the Ornstein-Uhlenbeck semigroup and its adjoint have come to play an important role in several branches of probability theory [HSU99] related, in some form, to Brownian motions. The fact that the explicitly known kernel (2) of the Fokker-Planck semigroup readily lends itself to analytical estimates has led to useful applications also outside the realm of probability theory. In particular, in recent years the Fokker-Planck semigroup has found applications in kinetic theory, the subfield of transport theory which is concerned with the approach to equilibrium and the response to driving external forces of individual continuum systems not in local thermal equilibrium; see, for instance, the review [Vil02].

However, the linear Fokker-Planck equation itself, (1), usually is not thought of as a kinetic equation for the particle density function on velocity space of an *individual, isolated* space-homogeneous system of particles in some compact domain, which perform a microscopic autonomous dynamics that may be deterministic or stochastic but should satisfy the usual conservation laws of mass (particle number), energy and, depending on the shape of the domain in physical space and its boundary conditions, also momentum and angular momentum. Evidently the very meaning of f and the parameters \mathbf{u} and T in (1) voids this interpretation. Yet, with a re-interpretation of f , \mathbf{u} and T it is possible to assign to (1) a kinetic meaning.

Incidentally, the first result showing that at least a partial re-interpretation of (1) in this direction is possible can be found in a paper by Villani [Vil98] who,

in his study of the space-homogeneous Landau equation for the weak deflection (i.e. Landau) limit of a gas of particles with Maxwellian molecular interactions, discovered that for isotropic velocity distribution functions f (and only for these) the Landau equation is identical to (1), with parameters $\mathbf{u} = \mathbf{0}$ and T matched to guarantee energy conservation. For general non-isotropic data the Landau equation for Maxwell molecules is identical to a more complicated equation than (1).

To pave the ground for a complete re-interpretation of (1), which requires re-assigning the meaning of f , \mathbf{u} and T , we first note that by the linearity of (1) we can scale f to any positive normalization we want. We now introduce the following functionals of f ,

the “mass of f ”

$$m(f) = \int_{\mathbb{R}^3} f(\mathbf{v}; t) d^3\mathbf{v}, \quad (3)$$

the “momentum of f ”

$$\mathbf{p}(f) = \int_{\mathbb{R}^3} \mathbf{v} f(\mathbf{v}; t) d^3\mathbf{v}, \quad (4)$$

and the “energy of f ”

$$e(f) = \int_{\mathbb{R}^3} \frac{1}{2} |\mathbf{v}|^2 f(\mathbf{v}; t) d^3\mathbf{v}. \quad (5)$$

The “angular momentum of f ” for a space-homogeneous $f(\mathbf{v}; t)$ is simply $\mathbf{j}(f) = \mathbf{x}_{\text{CM}} \times \mathbf{p}(f)$, with \mathbf{x}_{CM} the center of mass of the system, but this does not add any further insight and hence will not be considered explicitly. The functionals (3), (4), and (5) inherit some time dependence from the solution $f(\cdot; t)$ of (1), but to find this dependence explicitly it is not necessary to solve for f first. Indeed, it is an elementary exercise in integration by parts to extract from (1) the following linear evolution equations with constant coefficients for m , \mathbf{p} , and e ,

$$\dot{m} = 0, \quad (6)$$

$$\dot{\mathbf{p}} = m\mathbf{u} - \mathbf{p}, \quad (7)$$

$$\dot{e} = 3T - 2e + \boldsymbol{u} \cdot \boldsymbol{p}, \tag{8}$$

which, beside the conservation of mass, i.e. $m(f) = m(f_0)$, describe the exponentially fast convergence to a stationary state $\mathbf{p}(f) \rightsquigarrow m(f_0)\mathbf{u}$ and $e(f) \rightsquigarrow \frac{3}{2}T + \frac{1}{2}m(f_0)|\mathbf{u}|^2$. While all this is of course quite trivial and well known, the relevant fact to realize here is that whenever the energy and the momentum of the initial f_0 equal these asymptotically stationary values, viz. if $\mathbf{p}(f_0) = m(f_0)\mathbf{u}$ and $e(f_0) = \frac{3}{2}T + \frac{1}{2}m(f_0)|\mathbf{u}|^2$, then beside mass m , also energy e and momentum \mathbf{p} will be conserved. Conservation of mass, energy, and momentum for such a large subset of initial data f_0 does not yet mean that we may already think of the linear equation (1) as a kinetic equation, which should conserve mass, energy, and (depending on the shape of the domain in physical space and its boundary conditions) also momentum for *all* initial data, no matter what their mass, energy and momentum are; moreover, a genuine kinetic equation for particles with (pair or higher order) interactions must express the time derivative of f in terms of an at least² bilinear operator in f . However, with the help of (3), (4) and (5) we now replace T and \mathbf{u} in (1) to obtain just such a kinetic equation.

Indeed, consider the *a priori* nonlinear Fokker–Planck equation

$$\partial_t f(\mathbf{v}; t) = \partial_{\mathbf{v}} \cdot \left(\frac{1}{3} (2e(f)m(f) - |\mathbf{p}(f)|^2) \partial_{\mathbf{v}} f(\mathbf{v}; t) + (m(f)\mathbf{v} - \mathbf{p}(f)) f(\mathbf{v}; t) \right), \quad (9)$$

where $f(\cdot; t) : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ now is a particle density function on velocity space at time $t \in \mathbb{R}_+$. The right-hand side of (9) is a sum of a bilinear and a trilinear operator acting on f which now guarantees conservation of mass, momentum, and energy for *all* initial data $f_0 \geq 0$, as verified by repeating the easy exercise in elementary integrations by parts using (9) to find $\dot{m} = 0$ as well as $\dot{\mathbf{p}} = m\mathbf{p} - \mathbf{p}m = \mathbf{0}$ and $\dot{e} = 2em - |\mathbf{p}|^2m - 2em + |\mathbf{p}|^2m = 0$. Of course, *after this fact* of mass, momentum, and energy conservations the *a priori* nonlinear equation (9) in effect becomes just a completely and explicitly solvable linear³ Fokker–Planck equation (1), only now with parameters \mathbf{u} and T which are not prescribed but determined through the

²The Boltzmann, the Landau, and the Vlasov kinetic equations have bilinear “interaction operators,” the Balescu–Lenard–Guernsey equation has a higher order nonlinearity which reduces to the bilinear format in the long wavelength regime.

³In this sense (9) is “almost nonlinear,” or “essentially linear,” depending on one’s viewpoint.

initial data f_0 , viz. $\mathbf{u} = \mathbf{p}(f_0)/m(f_0) \equiv \mathbf{u}_0$ and $\frac{3}{2}T = e(f_0) - |\mathbf{p}(f_0)|^2/2m(f_0) \equiv \varepsilon_0$; we also set $m(f_0) \equiv m_0$ and $e(f_0) = e_0$. Accordingly, (9) inherits from (1) the feature that, as $t \rightarrow \infty$, its solutions f converge pointwise exponentially fast to the Maxwellian equilibrium state

$$f_M(\mathbf{v}) = m_0 \left(\frac{3}{4\pi\varepsilon_0} \right)^{\frac{3}{2}} \exp \left(-\frac{3|\mathbf{v} - \mathbf{u}_0|^2}{4\varepsilon_0} \right), \quad (10)$$

with monotonically increasing relative entropy

$$S(f|f_M) = - \int_{\mathbb{R}^3} f(\mathbf{v}; t) \ln \frac{f(\mathbf{v}; t)}{f_M(\mathbf{v})} d^3\mathbf{v} \quad (11)$$

which in fact approaches its maximum value 0 exponentially fast.

Since (9) displays all the familiar features of a kinetic equation (formal nonlinearity; conservation laws of mass, momentum, energy; an H -Theorem; approach to equilibrium; Maxwellian equilibrium states), at this point we may legitimately contemplate (9) as a kinetic equation of some spatially homogeneous, isolated system of N interacting particles in a compact spatial domain compatible with momentum conservation (e.g. a rectangle with periodic boundary conditions). In the remainder of this paper we show explicitly how (9) arises from the Kolmogorov equation⁴ for the adjoint evolution of an underlying N -particle Markov process in the limit $N \rightarrow \infty$. We use the strategy originally introduced by Kac [Kac56] in 1956 in the context of his work on a caricature of the Boltzmann equation; for important recent work on Kac's original program, see [CCL02]. As Kac realized, the crucial property that needs to be established in order to validate the $N \rightarrow \infty$ limit is what he called "propagation of chaos," which loosely speaking means that if the particle velocities are uncorrelated at $t = 0$, they remain uncorrelated at later times; this can be rigorously true only on the continuum scale in the limit $N \rightarrow \infty$.

Interestingly enough, by adding some suitable lower order terms to the putatively simplest N -particle Markov process that leads to the (kinetic) Fokker-Planck equation in the limit $N \rightarrow \infty$, the corresponding Kolmogorov equation for an ensemble of such isolated N -particle systems can be simplified to be just the diffusion

⁴In the physics literature, the Kolmogorov equation for an N -particle Markov process is traditionally called "master equation".

equation on the $3N - 4$ -dimensional manifold (a sphere) of constant energy and momentum. Since therefore both the finite- N and the infinite- N equations are exactly solvable, the kinetic limit $N \rightarrow \infty$ can be carried out explicitly and studied in great detail. For this reason we actually defer the discussion of the underlying N -particle process to Appendix Ab while in the main part of our paper we analyse the diffusion equation on $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ and derive from it the kinetic Fokker–Planck equation on \mathbb{R}^3 .

Technically, we apply the Laplace–Beltrami operator to a probability density on $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ and then integrate out $N - n$ velocities over their constrained domain of accessibility. Taking next the limit $N \rightarrow \infty$ yields a Fokker–Planck operator acting on the n -th marginal density on \mathbb{R}^{3n} . Thus we obtain a linear Fokker–Planck hierarchy of equations indexed by n . Using the Hewitt–Savage decomposition theorem, the hierarchy is seen to be generated by the single, *a priori* nonlinear kinetic Fokker–Planck equation (9) which in view of the conservation laws is equivalent to the essentially linear Fokker–Planck equation (1) with constant parameters which are determined by the initial data.

Experts in probability theory may have noticed a similarity between the first part of our program and what has been called the “Poincaré limit” [Bak02]; in fact, our approach is “dual” to Bakry’s approach. More specifically, Bakry [Bak02] has shown that the action of the Laplace–Beltrami operator for $\mathbb{S}_{\sqrt{N}}^N \hookrightarrow \mathbb{R}^{N+1}$ on a probability density function over a “radial” coordinate axis of $\mathbb{S}_{\sqrt{N}}^N$ becomes identical, in the limit $N \rightarrow \infty$, to the action of the Ornstein–Uhlenbeck operator on the same density viewed as a function over \mathbb{R} . Obviously, whenever the “radial” function is obtained by taking the marginal of a probability density over $\mathbb{S}_{\sqrt{N}}^N$, i.e. by integrating out the $N - 1$ Cartesian coordinates of the embedding space which are perpendicular to a fixed “radial” direction, the Ornstein–Uhlenbeck operator acts on the limiting marginal density as $N \rightarrow \infty$. This relationship between the operators is reflected at the spectral level by the convergence of the whole structure of orthogonal eigenfunctions of the Laplacian on $\mathbb{S}_{\sqrt{N}}^N$ (hyper-spherical harmonics) to the orthogonal eigenfunctions of the Ornstein–Uhlenbeck operator on \mathbb{R} (Hermite

polynomials multiplied by the square root of their Gaussian weight function); one of the earliest works is [Meh66], while more recent works on the Poincaré limit, containing interesting connections with the theory of Markov semigroups, are [Bak02] and [BaMa03]. Our procedure is “dual” to Bakry’s approach in the sense that we integrate out subsets of the Cartesian variables of the embedding space *after* having applied the Laplace–Beltrami operator to a probability density on the high-dimensional sphere, thereby obtaining the *adjoint* Ornstein–Uhlenbeck operator acting on the respective marginals; in addition, while Bakry considers only mass and energy conservation, we consider conservation of mass, energy, and momentum.

Incidentally, our work is not inspired by Bakry’s works on the Poincaré limit, nor by Villani’s discovery about the isotropic evolution of the space-homogeneous Landau equation, about both of which we learned only after our own findings. Rather, our study of the diffusion equations on the $3N - C$ -dimensional spheres of constant energy ($C = 1$), respectively energy and momentum ($C = 4$), which began in [KiLa04], was originally conceived of as a *technically simpler primer* for our investigation (also in [KiLa04]) of the Balescu–Prigogine master equation for Landau’s kinetic equation. And while the present paper is also a technical continuation of [KiLa04], in the sense that here we supply various calculations that we had announced in [KiLa04], the main purpose of the present paper is to amplify the conceptual spin-off of our technical investigations, the *new physical interpretation* of one of the simplest and best known linear transport equations as an (almost nonlinear) kinetic equation. As should be clear from our discussion in this introduction, this kinetic theory interpretation of the prototype Fokker–Planck equation may have been suspected by others long ago, yet we have not been able to find the whole story in the literature.

In what follows, for the sake of simplicity we set $m_0 = 1$, and accordingly⁵ obtain $\mathbf{p}(f_0) \equiv \mathbf{u}_0$ and $e(f_0) - |\mathbf{p}(f_0)|^2/2 = e_0 - |\mathbf{u}_0|^2/2 \equiv \varepsilon_0$. With these simplifications

⁵Setting $m_0 = 1$ means we should now speak of the energy per particle e_0 , the thermal energy per particle ε_0 , and the momentum per particle $\mathbf{p}_0 (= \mathbf{u}_0)$.

(9) now becomes

$$\partial_t f(\mathbf{v}; t) = \partial_{\mathbf{v}} \cdot \left(\frac{2}{3} \varepsilon_0 \partial_{\mathbf{v}} f(\mathbf{v}; t) + (\mathbf{v} - \mathbf{u}_0) f(\mathbf{v}; t) \right). \quad (12)$$

While (12) is essentially a linear PDE, it should just be kept in mind that ε_0 and \mathbf{u}_0 are functionals of f which are determined by the initial data f_0 and not chosen independently.⁶ We next shall derive (12) from the diffusion equation on $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ in the spirit of Kac's program.

2 The Finite- N Ensembles

Consider an infinite ensemble of i.i.d. random vectors $\{\mathbf{V}_\alpha\}_{\alpha=1}^\infty$ where each $\mathbf{V} = (\mathbf{v}_1, \dots, \mathbf{v}_N) \in \mathbb{R}^{3N}$ represents a possible micro-state of an individual system of N particles with velocities $\mathbf{v}_i = (v_{i1}, v_{i2}, v_{i3}) \in \mathbb{R}^3$ and particle positions assumed to be uniformly distributed over a periodic box; hence, particle positions will not be considered explicitly. Each \mathbf{V} takes values in the $3N - 4$ -dimensional manifold of constant energy e_0 and momentum \mathbf{u}_0 ,

$$\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4} = \left\{ \mathbf{V} : \sum_{k=1}^N \mathbf{v}_k = N\mathbf{u}_0, \sum_{k=1}^N \frac{1}{2} |\mathbf{v}_k|^2 = Ne_0, e_0 > \frac{1}{2} |\mathbf{u}_0|^2 \right\}. \quad (13)$$

The manifold $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ is identical to a $3N - 4$ -dimensional sphere of radius $\sqrt{2N\varepsilon_0}$ (where ε_0 appears above (12)), centered at $\mathbf{U} = (\mathbf{u}_0, \dots, \mathbf{u}_0)$ and embedded in the $3(N - 1)$ -dimensional affine linear subspace of \mathbb{R}^{3N} given by $\mathbf{U} + \mathbb{L}^{3N-3}$, where $\mathbb{L}^{3N-3} \equiv \mathbb{R}^{3N} \cap \{\mathbf{V} \in \mathbb{R}^{3N} : \sum_{k=1}^N \mathbf{v}_k = \mathbf{0}\}$ is the space of velocities in any center-of-mass frame. The ensemble at time τ is characterized by a probability density $F^{(N)}(\mathbf{V}; \tau)$ on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$, the evolution of which is determined by the diffusion equation

$$\partial_\tau F^{(N)}(\mathbf{V}; \tau) = \Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}} F^{(N)}(\mathbf{V}; \tau), \quad (14)$$

where $\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ is the Laplace–Beltrami operator on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$. Since all particles are of the same kind, we consider only solutions to (14) which are invariant under the

⁶The identification of (9) with (12) is valid only for isolated systems that can freely translate. If a driving external force field \mathbf{F} is applied, then $e(f)$ and $\mathbf{p}(f)$ are no longer constant and (9) – with the addition of the forcing term $-\mathbf{F} \cdot \partial_{\mathbf{v}} f$ to its r.h.s. – is the relevant equation.

symmetric group S_N applied to the N components in \mathbb{R}^3 of \mathbf{V} . Clearly, permutation symmetry is preserved by the evolution.⁷ We will show that the diffusion equation (14), here viewed as a master equation, leads precisely to the essentially linear Fokker–Planck equation (12) in the sense of Kac’s program: (a) the Fokker–Planck equation (12) arises as the $N \rightarrow \infty$ limit of the equation for the first marginal of $F^{(N)}(\mathbf{V}; \tau)$ derived from (14), and (b) propagation of chaos holds. In this section we prepare the ground by discussing the finite- N equation (14). The limit $N \rightarrow \infty$ is carried out in the next section, while propagation of chaos is discussed in the final section.

For the sake of completeness, we begin by listing some general facts about the diffusion equation. We note that the Laplacian $\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ is a positive semi-definite, essentially self-adjoint operator on the dense domain $\mathfrak{C}^\infty(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}) \subset \mathfrak{L}^2(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$, thus it has a unique self-adjoint extension with domain $\mathfrak{H}^2(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$. Its self-adjoint extension is the generator of a non-expansive semigroup on $\mathfrak{L}^2(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$ which is strictly contracting on the \mathfrak{L}^2 orthogonal complement of the constant functions. Thus, we may ask that the initial condition $\lim_{t \downarrow 0} F^{(N)}(\cdot; \tau) = F_0^{(N)}(\cdot) \in \mathfrak{L}^2(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$ (which implies $F_0^{(N)} \in \mathfrak{L}^1(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$). Yet, as is well-known, the diffusion semigroup is so strongly regularizing that we may even take $F_0^{(N)}(\cdot) \in \mathfrak{M}_{+,1}(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$, a probability measure, and obtain $F^{(N)}(\cdot; \tau) \in \mathfrak{C}^\infty(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$ for all $\tau > 0$.

In fact, the solutions of (14) can be computed quite explicitly in terms of an eigenfunction expansion. Since via translation by \mathbf{U} (choosing a center-of-mass frame) and scaling by $\sqrt{2N\varepsilon_0}$ (choosing a convenient unit of energy) the manifold $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ can be identified with the unit sphere centered at the origin of the linear subspace $\mathbb{L}^{3N-3} \subset \mathbb{R}^{3N}$, the complete spectrum of $\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ and an orthogonal basis of eigenfunctions can be obtained from the well-known eigenvalues and eigenfunctions for the Laplacian on the unit sphere $\mathbb{S}^{3N-4} \hookrightarrow \mathbb{R}^{3N-3}$. Of course, in our

⁷In what follows, for the sake of notational simplicity we will not enforce this symmetry explicitly, but the reader should be aware that (for instance) all the eigenfunctions that appear below in the solution for $F^{(N)}$ can be easily symmetrized.

case the embedding is $\mathbb{S}^{3N-4} \hookrightarrow \mathbb{L}^{3N-3}$ with \mathbb{L}^{3N-3} isomorphic by a rotation to standard \mathbb{R}^{3N-3} . Thus we start from $\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}$ and we first carry out a rotation in \mathbb{R}^{3N} that transforms \mathbf{V} to $\mathbf{W} = \mathcal{U}\mathbf{V}$ in such a way that \mathbb{L}^{3N-3} is mapped to the $3N-3$ -dimensional linear subspace $\{\mathbf{W} : \mathbf{w}_N = \mathbf{0}\}$. Obviously, \mathcal{U}^T is the linear transformation that diagonalizes the projection operator onto \mathbb{L}^{3N-3} . A complete orthonormal set of eigenvectors for such a projection is readily calculated and leads to

$$\begin{aligned}
\mathbf{w}_1 &= \sqrt{\frac{N-1}{N}} \left[\mathbf{v}_1 - \frac{1}{N-1} \sum_{i=2}^N \mathbf{v}_i \right] \\
&\vdots \\
\mathbf{w}_n &= \sqrt{\frac{N-n}{N-n+1}} \left[\mathbf{v}_n - \frac{1}{N-n} \sum_{i=n+1}^N \mathbf{v}_i \right] \\
&\vdots \\
\mathbf{w}_{N-1} &= \frac{1}{\sqrt{2}} [\mathbf{v}_{N-1} - \mathbf{v}_N] \\
\mathbf{w}_N &= \frac{1}{\sqrt{N}} \sum_{i=1}^N \mathbf{v}_i
\end{aligned} \tag{15}$$

It is easily checked that the matrix associated with this transformation is indeed orthogonal, and that \mathbf{w}_N vanishes whenever $\mathbf{V} \in \mathbb{L}^{3N-3}$. More generally, the affine subspace $\mathbf{U} + \mathbb{L}^{3N-3}$ is mapped to the linear manifold $\{\mathbf{W} : \mathbf{w}_N = \sqrt{N}\mathbf{u}_0\}$ and $\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}$ is mapped to

$$\left\{ \mathbf{W} : \mathbf{w}_N = \sqrt{N}\mathbf{u}_0, \quad \sum_{i=1}^{N-1} |\mathbf{w}_i|^2 = 2N\varepsilon_0 - N|\mathbf{u}_0|^2 = 2N\varepsilon_0 \right\} \tag{16}$$

which implies that the truncated vector $(\mathbf{w}_1, \dots, \mathbf{w}_{N-1})$ belongs to the sphere $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4} \hookrightarrow \mathbb{R}^{3N-3}$ (in \mathbf{w}_k -coordinates). Thus, the transform \mathcal{U} allows one to analyse the N -particle system with energy and momentum conservation (“periodic box” setup) in terms of an $(N-1)$ -particle system with only energy conservation (a “container with reflecting walls” setup).⁸ For future reference, we also observe that for n fixed and $N \rightarrow \infty$ the effect of \mathcal{U} reduces to a translation of each of the n ve-

⁸The gas in such a container was discussed in our earlier work [KiLa04], but without detailed calculations. Our calculations with the \mathbf{w} variables here now supply the relevant details.

locities by \mathbf{u}_0 , in the following sense. Consider a consistent hierarchy of vectors of increasing size N , in which lower- N vectors can be obtained from the higher- N ones by truncation (i.e. projection). Suppose that the vectors belong to $\mathbf{U} + \mathbb{L}^{3N-3}$ for all N , apply the transformation in (15) and look at the n -th component. Since $\sum_{i=n+1}^N \mathbf{v}_i = N\mathbf{u}_0 - \sum_{i=1}^n \mathbf{v}_i$, where $\sum_{i=1}^n \mathbf{v}_i$ is independent of N , we find

$$\lim_{N \rightarrow \infty} \mathbf{w}_n = \mathbf{v}_n - \mathbf{u}_0. \quad (17)$$

We now recall that the Laplacian is invariant under Euclidean transformations. Thus, under our orthogonal transformation \mathcal{U} , the Laplacian $\Delta_{\mathbb{M}_{\mathbf{u}_0, \mathbf{e}_0}^{3N-4}}$ becomes the Laplacian on $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ in \mathbb{R}^{3N-3} , the space of truncated vectors $(\mathbf{w}_1, \dots, \mathbf{w}_{N-1})$ (which will also be denoted by \mathbf{W} , at the price of abusing the notation). Since $\Delta_{\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}} = \frac{1}{2N\varepsilon_0} \Delta_{\mathbb{S}^{3N-4}}$, and the Laplacian on the unit sphere \mathbb{S}^{3N-4} has spectrum $j(j+3N-5)$, $j = 0, 1, \dots$, the spectrum of $\Delta_{\mathbb{M}_{\mathbf{u}_0, \mathbf{e}_0}^{3N-4}}$ is

$$\lambda_{\mathbb{M}_{\mathbf{u}_0, \mathbf{e}_0}^{3N-4}}^{(j)} = \frac{j(j+3N-5)}{2N\varepsilon_0}, \quad j = 0, 1, \dots \quad (18)$$

The eigenspace on \mathbb{S}^{3N-4} for the j -th eigenvalue has dimension

$$\mathcal{N}(j, 3N-3) = \frac{(3N-5+2j)(3N-6+j)!}{j!(3N-5)!} \quad (19)$$

and is spanned by an orthogonal basis of hyper-spherical harmonics⁹ on $\mathbb{S}^{3N-4} \subset \mathbb{R}^{3N-3}$ of order j , here denoted $\tilde{Y}_{j,\ell}(\boldsymbol{\omega}; 3N-3)$, with $\ell \in \mathbb{D}_j = \{1, \dots, \mathcal{N}(j, 3N-3)\}$ and with $\boldsymbol{\omega} \in \mathbb{S}^{3N-4}$. The indexing of our $\tilde{Y}_{j,\ell}(\boldsymbol{\omega}; 3N-3)$ follows the convention of [Mül98] for his $Y_{j,\ell}$ and differs from what might have been anticipated from the familiar convention for spherical harmonics on \mathbb{S}^2 . Our reason for using tildes atop the function symbols is to remind the reader that we will use a normalization of the $\tilde{Y}_{j,\ell}(\boldsymbol{\omega}; 3N-3)$ which conveniently suits our purposes and does not seem to agree with any of the existing conventions, such as in [Mül98] or for the spherical harmonics on \mathbb{S}^2 . Our convention is motivated by the analysis of the large N behavior of the eigenfunctions, carried out in Appendix B.

⁹The hyper-spherical harmonics on \mathbb{S}^n are restrictions to $\mathbb{S}^n \subset \mathbb{R}^{n+1}$ of homogeneous harmonic polynomials in \mathbb{R}^{n+1} . For $j > 0$ the restriction has to be non-constant, since $\tilde{Y}_{0,1} \equiv \text{const.}$

Hence, the eigenspace of $\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ associated with the j -th eigenvalue in (18) is spanned by the eigenfunctions $\tilde{Y}_{j,\ell}(\mathbf{W}/\sqrt{2N\varepsilon_0}; 3N-3)$, $\ell \in \mathbb{D}_j$, where \mathbf{W} is given by (15) for $n = 1, \dots, N-1$. To shorten the notation we introduce

$$G_{j,\ell}^{(N)}(\mathbf{V}) \equiv |\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}|^{-1} \tilde{Y}_{j,\ell}(\mathbf{W}/\sqrt{2N\varepsilon_0}; 3N-3); \quad (20)$$

here, the factor $|\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}|^{-1}$ is introduced for later convenience.

In terms of the eigenfunctions $G_{j,\ell}^{(N)}(\mathbf{V})$, the solution to equation (14) is simply given by the generalized Fourier series

$$F^{(N)}(\mathbf{V}; \tau) = |\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}|^{-1} + \sum_{j \in \mathbb{N}} \sum_{\ell \in \mathbb{D}_j} F_{j,\ell}^{(N)} G_{j,\ell}^{(N)}(\mathbf{V}) e^{-\frac{j(j+3N-5)}{2N\varepsilon_0} \tau} \quad (21)$$

with Fourier coefficients $F_{j,\ell}^{(N)}$ given by

$$F_{j,\ell}^{(N)} = \frac{\langle F_0^{(N)} | G_{j,\ell}^{(N)} \rangle}{\langle G_{j,\ell}^{(N)} | G_{j,\ell}^{(N)} \rangle} \quad (22)$$

where $\langle \cdot | \cdot \rangle$ denotes the inner product in $\mathcal{L}^2(\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4})$. Notice, though, that the numerator $\langle F_0^{(N)} | G_{j,\ell}^{(N)} \rangle$ can be extended to mean the canonical pairing of the $G_{j,\ell}^{(N)}$ s with an element of their dual space, which allows us to take $F_0^{(N)}$ to be a measure. In particular, we may take $F_0^{(N)}$ to be the Dirac measure concentrated at any particular point of $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$. The formula (21) then describes the fundamental solution of the diffusion equation (14). In any event, whatever $F_0^{(N)}$, (21) makes it evident that when $\tau \rightarrow \infty$ the ensemble probability density function on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ decays exponentially fast to the uniform probability density $|\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}|^{-1} = |\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}|^{-1} = F_{0,1}^{(N)} G_{0,1}^{(N)}(\mathbf{V})$, which is the constant eigenfunction corresponding to the smallest non-degenerate eigenvalue 0 of the Laplacian.

3 Evolution of the Marginals

To study the limit $N \rightarrow \infty$ for the time-evolution of the ensemble measure, we need to consider the hierarchy of n -velocity marginal distributions

$$F^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) \equiv \int_{\Omega_{\mathbf{u}_0, e_0}^{3(N-n)-4}} F^{(N)}(\mathbf{V}; \tau) d\mathbf{v}_{n+1} \dots d\mathbf{v}_N \quad (23)$$

where $\Omega_{\mathbf{u}_0, e_0}^{3(N-n)-4}$ is given by all the $(\mathbf{v}_{n+1}, \dots, \mathbf{v}_N)$ such that

$$\sum_{i=n+1}^N \mathbf{v}_i = N\mathbf{u}_0 - \sum_{i=1}^n \mathbf{v}_i, \quad \sum_{i=n+1}^N |\mathbf{v}_i|^2 = 2Ne_0 - \sum_{i=1}^n |\mathbf{v}_i|^2 \quad (24)$$

and $F^{(n|N)}$ has domain $\{(\mathbf{v}_1, \dots, \mathbf{v}_n) : \sum_{k=1}^n |\mathbf{v}_k - \mathbf{u}_0|^2 \leq 4(N-n)\varepsilon_0\} \subset \mathbb{R}^{3n}$.

The evolution equation for the n -th marginal $F^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau)$ is obtained by integrating (14) over $(\mathbf{v}_{n+1}, \dots, \mathbf{v}_N) \in \mathbb{R}^{3N-3n}$, using the representation of the Laplace–Beltrami operator given in (49) of Appendix Aa. Then, a straightforward calculation (previously presented in [KiLa04]) shows that $F^{(n|N)}$ satisfies

$$\begin{aligned} \partial_\tau F^{(n|N)} &= \sum_{i=1}^n \frac{\partial}{\partial \mathbf{v}_i} \cdot \frac{\partial F^{(n|N)}}{\partial \mathbf{v}_i} - \frac{1}{N} \sum_{k=1}^3 \sum_{i,j=1}^n \frac{\partial^2 F^{(n|N)}}{\partial v_{ik} \partial v_{jk}} \\ &\quad - \frac{1}{2N\varepsilon_0} \sum_{i,j=1}^n \frac{\partial}{\partial \mathbf{v}_i} \cdot \left((\mathbf{v}_i - \mathbf{u}_0)(\mathbf{v}_j - \mathbf{u}_0) \cdot \frac{\partial F^{(n|N)}}{\partial \mathbf{v}_j} \right) \\ &\quad + \frac{3(N-n)}{2\varepsilon_0 N} \sum_{i=1}^n \frac{\partial}{\partial \mathbf{v}_i} \cdot \left((\mathbf{v}_i - \mathbf{u}_0) F^{(n|N)} \right). \end{aligned} \quad (25)$$

Clearly, to obtain the solutions of these equations it is advisable to integrate the series solution for $F^{(N)}(\mathbf{V}; \tau)$, (21). For this purpose, it will be convenient to calculate the marginals in terms of the rotated variables \mathbf{W} . Changing the integration variables¹⁰ gives

$$F^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) = \sqrt{\frac{N}{N-n}} \int F^{(N)}(\mathbf{V}; \tau) d\mathbf{w}_{n+1} \dots d\mathbf{w}_{N-1} \quad (26)$$

where the integral is over $\mathbb{S}^{\frac{3(N-n)-4}{\sqrt{2N\varepsilon_0 - \sum_{i=1}^n |\mathbf{w}_i|^2}}}$, and we abused the notation $F^{(N)}(\mathbf{V}; \tau)$ by applying it to what is now regarded as a function of $(\mathbf{v}_1, \dots, \mathbf{v}_n, \mathbf{w}_{n+1}, \dots, \mathbf{w}_{N-1})$.

To obtain the series solution for $F^{(n|N)}(\mathbf{V}; \tau)$ we need to express (21) in the variables $(\mathbf{v}_1, \dots, \mathbf{v}_n, \mathbf{w}_{n+1}, \dots, \mathbf{w}_{N-1})$ and then integrate term by term in the spirit of (26). To accomplish this we need to choose explicitly a basis of spherical harmonics $\tilde{Y}_{j,\ell}$ on \mathbb{S}^{3N-4} . It is convenient to do this in an iterative fashion, by assuming that a basis is known for the spherical harmonics with one independent variable less, here $\tilde{Y}_{k,m}(\boldsymbol{\omega}_{3N-5}; 3N-4)$ with $\boldsymbol{\omega}_{3N-5} \in \mathbb{S}^{3N-5}$. Then, the desired basis is obtained [Mül98] by taking all the elements in the given lower-dimensional basis and

¹⁰Note that (15) defines a one-to-one linear map with determinant $\sqrt{\frac{N}{N-n}}$ between $(\mathbf{v}_{n+1}, \dots, \mathbf{v}_N)$ and $(\mathbf{w}_{n+1}, \dots, \mathbf{w}_{N-1}, \mathbf{z}_N)$, where $\mathbf{z}_N \equiv \mathbf{w}_N - \frac{1}{\sqrt{N}} \sum_{i=1}^n \mathbf{v}_i$.

multiplying them by associated Legendre functions of the “extra” variable. In our case the $(3N-3)$ -th variable will be $w_{11}/\sqrt{2N\varepsilon_0}$, the first component of $\mathbf{W}/\sqrt{2N\varepsilon_0}$, and $\boldsymbol{\omega}_{3N-5}$ will be a unit vector in the space of the remaining $3N-4$ components, denoted by $(\mathbf{W})_{3N-4}/\sqrt{2N\varepsilon_0}$; thus,

$$\tilde{Y}_{j,\ell} \left(\frac{\mathbf{W}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) = \tilde{Y}_{k,m} \left(\frac{(\mathbf{W})_{3N-4}}{\sqrt{2N\varepsilon_0}}; 3N-4 \right) \tilde{P}_j^k \left(\frac{w_{11}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) \quad (27)$$

where $k = 0, 1, \dots, j$, $m = 1, \dots, \mathcal{N}(k, 3N-4)$ and each choice of the pair k, m is associated with a value of the degeneracy index ℓ for the basis $\tilde{Y}_{j,\ell}$; moreover, \tilde{P}_j^k is an associated Legendre function [Mül98], suitably normalized (see Appendix B).

By repeating this process $3n$ times, we write out the eigenfunctions in the form

$$\begin{aligned} \tilde{Y}_{j,\ell} \left(\frac{\mathbf{W}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) &= \tilde{Y}_{k_{3n},m} \left(\frac{(\mathbf{W})_{3N-3n-3}}{\sqrt{2N\varepsilon_0}}; 3N-3n-3 \right) \times \\ &\times \tilde{P}_{k_{3n-1}}^{k_{3n}} \left(\frac{w_{n3}}{\sqrt{2N\varepsilon_0}}; 3N-3n-2 \right) \tilde{P}_{k_1}^{k_2} \left(\frac{w_{12}}{\sqrt{2N\varepsilon_0}}; 3N-4 \right) \dots \tilde{P}_j^{k_1} \left(\frac{w_{11}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) \end{aligned} \quad (28)$$

where $0 \leq k_{3n} \leq \dots \leq k_1 \leq j$ and $m = 1, \dots, \mathcal{N}(k_{3n}, 3N-3n-3)$. Now let $g_{j,\ell}^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n)$ denote the n -th “marginal” of $G_{j,\ell}^{(N)}(\mathbf{V})$ (as for $F^{(N)}$ in (26)), and set $N^* \equiv N - n - 1$. We find

$$\begin{aligned} g_{j,\ell}^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n) &= |\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}|^{-1} \int \tilde{Y}_{k_{3n},m} \left(\frac{(\mathbf{W})_{3N^*}}{\sqrt{2N\varepsilon_0}}; 3N^* \right) d\mathbf{w}_{n+1} \dots d\mathbf{w}_{N-1} \\ &\times \sqrt{\frac{N}{N-n}} \tilde{P}_{k_{3n-1}}^{k_{3n}} \left(\frac{w_{n3}}{\sqrt{2N\varepsilon_0}}; 3N-3n-2 \right) \dots \tilde{P}_j^{k_1} \left(\frac{w_{11}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) \end{aligned} \quad (29)$$

where the integral is over the same domain as in (26). The integral of $\tilde{Y}_{k_{3n},m}$ is non-zero if and only if $k_{3n} = 0$ and $m = 1$, and the integrals over $\tilde{Y}_{0,1}$ are determined only up to the overall factor $\tilde{Y}_{0,1}$, which we may choose to be unity without loss of generality. Accordingly, $g_{j,\ell}^{(n|N)} \equiv 0$ unless $\ell \in \tilde{\mathbb{D}}_j \subset \mathbb{D}_j$, where $\tilde{\mathbb{D}}_j$ contains the indices of the basis functions that “descend” from the uniform harmonic in $\mathbb{R}^{3N-3n-3}$. For such ℓ ’s the integrated eigenfunctions then become

$$\begin{aligned} g_{j,\ell}^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n) &= \tilde{P}_j^{k_1} \left(\frac{w_{11}}{\sqrt{2N\varepsilon_0}}; 3N-3 \right) \dots \tilde{P}_{k_{3n-1}}^0 \left(\frac{w_{n3}}{\sqrt{2N\varepsilon_0}}; 3N-3n-2 \right) \\ &\times \sqrt{\frac{N}{N-n}} \frac{|\mathbb{S}^{3(N-n)-4}|}{|\mathbb{S}^{3N-4}|} \frac{1}{\sqrt{2N\varepsilon_0}^{3n}} \left(1 - \frac{1}{\sqrt{2N\varepsilon_0}} \sum_{i=1}^n |\mathbf{w}_i|^2 \right)^{\frac{3(N-n)-4}{2}}. \end{aligned} \quad (30)$$

The series for the n -th marginal $F^{(n|N)}(\cdot; \tau)$ (the integrated (21)) is a series in the functions (30), viz.

$$F^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) = \sum_{j \in \mathbb{N} \cup \{0\}} \sum_{\ell \in \mathbb{D}_j} F_{j,\ell}^{(N)} g_{j,\ell}^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n) e^{-\frac{j(j+3N-5)}{2N\varepsilon_0} \tau}. \quad (31)$$

4 The Limit $N \rightarrow \infty$

We are now ready to take the infinitely many particles limit. First of all, we observe that the evolution equation for the marginal velocity densities $f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) \equiv \lim_{N \rightarrow \infty} F^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau)$ which obtains in the formal limit $N \rightarrow \infty$ from (25) is the essentially linear Fokker–Planck equation in \mathbb{R}^{3n} ,

$$\partial_\tau f^{(n)} = \sum_{i=1}^n \frac{\partial}{\partial \mathbf{v}_i} \cdot \left(\frac{\partial f^{(n)}}{\partial \mathbf{v}_i} + \frac{3}{2\varepsilon_0} (\mathbf{v}_i - \mathbf{u}_0) f^{(n)} \right). \quad (32)$$

We now show that the series expansion for the time-evolved finite- N marginals $F^{(n|N)}(\cdot; \tau)$ converge under natural conditions to solutions of these equations.

Beginning with the spectrum of $\Delta_{\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}}$, we note that the limit $N \rightarrow \infty$ yields

$$\lim_{N \rightarrow \infty} \left\{ \lambda_{\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}}^{(j)} \right\}_{j=0}^\infty = \left\{ \frac{3j}{2\varepsilon_0} \right\}_{j=0}^\infty. \quad (33)$$

Thus, the limit spectrum is discrete. In particular, there is a spectral gap separating the origin from the rest of the spectrum. As a result, the time evolution of the limit $N \rightarrow \infty$ continues to approach a stationary state exponentially fast when $\tau \rightarrow \infty$.

Coming to the eigenfunctions, the expression on the second line in (30) contains the n -velocity marginal distribution of the uniform density $|\mathbb{M}_{\mathbf{u}_0, \varepsilon_0}^{3N-4}|^{-1}$ (the $j = 0$ case). As is well-known at least since the time of Boltzmann, this distribution converges pointwise when $N \rightarrow \infty$ to the n -velocity drifting Maxwellian on \mathbb{R}^{3n} ,

$$f_M^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) = \left(\frac{3}{4\pi\varepsilon_0} \right)^{\frac{3n}{2}} \prod_{i=1}^n \exp \left(-\frac{3}{4\varepsilon_0} |\mathbf{v}_i - \mathbf{u}_0|^2 \right) \quad (34)$$

(recall (17)). In terms of eigenfunctions this means that the “projection” onto \mathbb{R}^{3n} of the $j = 0$ eigenfunction of the Laplace–Beltrami operator on $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ converges pointwise (in fact, even uniformly) to the $j = 0$ eigenfunction of the linear Fokker–Planck operator in \mathbb{R}^{3n} , appearing in the r.h.s. of (32). The connection between

the eigenfunctions generalizes to the cases $j \neq 0$; cf. [BaMa03] for the special case $\mathbf{u}_0 = \mathbf{0}$. The asymptotic behavior for $N \rightarrow \infty$ of the associated Legendre functions in (30), which is discussed in Appendix B, together with (17), yields that $g_{j,\ell}^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n) \equiv \lim_{N \rightarrow \infty} g_{j,\ell}^{(n|N)}(\mathbf{v}_1, \dots, \mathbf{v}_n)$ exists pointwise for all $(\mathbf{v}_1, \dots, \mathbf{v}_n) \in \mathbb{R}^{3n}$, with

$$\begin{aligned} g_{j,\ell}^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n) &= \frac{(-1)^j}{2^{j/2}} H_{j-k_1} \left(\sqrt{\frac{3}{4\varepsilon_0}} (v_{11} - u_1) \right) \cdots H_{k_{3n-1}} \left(\sqrt{\frac{3}{4\varepsilon_0}} (v_{n3} - u_3) \right) \\ &\quad \times \left(\frac{3}{4\pi\varepsilon_0} \right)^{\frac{3n}{2}} \prod_{i=1}^n \exp \left(-\frac{3}{4\varepsilon_0} |\mathbf{v}_i - \mathbf{u}_0|^2 \right) \\ &\equiv \frac{(-1)^j}{2^{j/2}} \left(\frac{3}{4\pi\varepsilon_0} \right)^{\frac{3n}{2}} \prod_{i=1}^n e^{-\frac{3}{4\varepsilon_0} |\mathbf{v}_i - \mathbf{u}_0|^2} \prod_{l=1}^3 H_{m_{i,l}} \left(\sqrt{\frac{3}{4\varepsilon_0}} (v_{il} - u_l) \right) \end{aligned} \quad (35)$$

for all $\ell \in \tilde{\mathbb{D}}_j$, where $H_m(x)$ is the Hermite polynomial of degree m on \mathbb{R} , and we defined $m_1 = j - k_1, m_2 = k_1 - k_2, \dots, m_{3n} = k_{3n-1}$. In terms of the m_i 's, the index set $\tilde{\mathbb{D}}_j$ counts all the choices of integers $0 \leq m_1, \dots, m_{3n} \leq j$ such that $\sum_{i=1}^{3n} m_i = j$. For $n = 1$ one readily recognizes the well-known eigenfunctions [Ris96] for the linear Fokker–Planck operator in \mathbb{R}^3 , viz. r.h.s.(12) with constant ε_0 and \mathbf{u}_0 , easily calculated by separation of variables. In fact, what we have recovered are precisely the eigenfunctions for the linear Fokker–Planck operator in \mathbb{R}^{3n} , see (32).

Now assume that one can choose sequences of initial conditions $F_0^{(N)}$ such that, for each fixed j and ℓ , the Fourier coefficients $F_{j,\ell}^{(N)}$ converge to a limit $F_{j,\ell}$ such that each initial n -velocity marginal density, $n \in \mathbb{N}$, converges in $(\mathfrak{L}^2 \cap \mathfrak{L}^1)(\mathbb{R}^{3n})$ to

$$f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; 0) = f_M^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) + \sum_{j \in \mathbb{N}} \sum_{\ell \in \tilde{\mathbb{D}}_j} F_{j,\ell} g_{j,\ell}^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n); \quad (36)$$

it then follows that the subsequent evolution of the n -velocity marginal densities is given by

$$f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) = f_M^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) + \sum_{j \in \mathbb{N}} \sum_{\ell \in \tilde{\mathbb{D}}_j} F_{j,\ell} g_{j,\ell}^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n) e^{-\frac{3j}{2\varepsilon_0} \tau}. \quad (37)$$

Formula (37) describes an exponentially fast approach to equilibrium in the ensemble of infinite systems. The $f^{(n)}(\cdot; \tau) \in (\mathfrak{L}^2 \cap \mathfrak{L}^1)(\mathbb{R}^{3n})$, and in addition they

automatically satisfy

$$\int_{\mathbb{R}^{3n}} f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) d\mathbf{v}_1 \dots d\mathbf{v}_n = 1 \quad (38)$$

$$\int_{\mathbb{R}^{3n}} (\mathbf{v}_1 + \dots + \mathbf{v}_n) f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) d\mathbf{v}_1 \dots d\mathbf{v}_n = n\mathbf{u}_0 \quad (39)$$

$$\int_{\mathbb{R}^{3n}} \frac{1}{2}(|\mathbf{v}_1|^2 + \dots + |\mathbf{v}_n|^2) f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) d\mathbf{v}_1 \dots d\mathbf{v}_n = ne_0 \quad (40)$$

for all $\tau \geq 0$ (recall that $e_0 = \varepsilon_0 + |\mathbf{u}|_0^2/2$). In fact, (37) solves (32), which now implies that $f^{(n)}(\cdot; \tau)$ can also be expressed through integration of the initial data against the n -fold tensor product of (2). The upshot is that $f^{(n)}(\cdot; \tau) \in \mathfrak{S}(\mathbb{R}^{3n}) \forall \tau > 0$ (Schwartz space). To vindicate these conclusions, for us it remains to show that the infinitely many constraints on each $F_{j,\ell}$ implied by (36), viz.

$$F_{j,\ell} = \frac{\langle f_0^{(n)} | g_{j,\ell}^{(n)} \rangle}{\langle g_{j,\ell}^{(n)} | g_{j,\ell}^{(n)} \rangle} \quad \forall n \in \mathbb{N}, \quad (41)$$

where $\langle \cdot | \cdot \rangle$ now means inner product in $\mathfrak{L}^2(\mathbb{R}^{3n})$, do not impose impossible consistency requirements. To show this, recall that the $f_0^{(n)}$ by definition satisfy

$$\int_{\mathbb{R}^3} f_0^{(n+1)}(\mathbf{v}_1, \dots, \mathbf{v}_{n+1}) d\mathbf{v}_{n+1} = f_0^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n), \quad (42)$$

which in view of (36) implies that the hierarchy of the $g_{j,\ell}^{(n)}$ must satisfy

$$\int_{\mathbb{R}^3} g_{j,\ell}^{(n+1)}(\mathbf{v}_1, \dots, \mathbf{v}_{n+1}) d\mathbf{v}_{n+1} = g_{j,\ell}^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n) \prod_{i=1}^3 \delta_{k_{3(n+1)-i}, 0}, \quad (43)$$

which is readily verified by explicit integration of (35). Thus, the constraints (41) are automatically consistent, and this vindicates our initial assumption.

5 Propagation of Chaos

Setting $n = 1$ in (32), and changing the time scale by setting $\tau = \frac{2}{3}\varepsilon_0 t$, we recover (12), with $f^{(1)}$ in place of f . However, (12) (or (9) for that matter) cannot be said to have been shown to be a kinetic equation yet. Note that propagation of chaos has not entered the derivation of (32). In fact, (32) for $n = 1, 2, \dots$ constitutes a “Fokker–Planck hierarchy” analogous to the the well-known Boltzmann, Landau

and Vlasov hierarchies which arise in the validation of kinetic theory [Spo91, CIP94] using ensembles. In our case the hierarchy has the very simplifying feature that the n -th equation in the hierarchy is decoupled from the equation for the $n + 1$ -th marginal. Since all the hierarchies used in the validation of kinetic theory are by construction *linear*¹¹ in the “vector” of the $f^{(n)}$, whenever one has a decoupling hierarchy one obtains closed linear equations for the $f^{(n)}$. In particular, our equation (32) with $n = 1$ is already a closed linear equation for $f^{(1)}$. However, at this point, any $f^{(n)}$ is still in general an ensemble superposition of states; in particular, $f^{(1)}$ still describes a statistical ensemble of pure states f with same mass, momentum, and energy. By ignoring this fact one can mislead oneself into thinking that (32) with $n = 1$ and $f^{(1)}$ in place of f is already the kinetic equation we sought.

The final step in extracting (12) as kinetic equation for the pure states involves the Hewitt–Savage [HeSa55] decomposition theorem. This theorem says that in the continuum limit any $f^{(n)}$ is a unique convex linear superposition of extremal (i.e. pure) n particle states, and that these pure states are products of n identical one-particle functions f evaluated at n generally different velocities. Each of the f in the support of the superposition measure represents the velocity density function of an actual individual member of the infinite statistical ensemble of infinitely-many-particles systems. In formulas, at $\tau = 0$ the initial data for $f^{(n)}$ read

$$f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; 0) = \langle f_0^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) \rangle, \quad (44)$$

where $\langle \cdot \rangle$ is the Hewitt–Savage [HeSa55] ensemble decomposition measure on the space of initial velocity density functions f_0 of individual physical systems with same mass $m(f_0) (= 1)$, momentum $\mathbf{p}(f_0) = \mathbf{u}_0$ and energy $e(f_0) = e_0 = \varepsilon_0 + |\mathbf{u}_0|^2/2$. To extend this representation to $\tau > 0$, let $U_\tau^{(n)}$ denote the one-parameter evolution semigroup for (32), i.e. $f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) = U_\tau^{(n)} f_0^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n)$. Noting now that the Hewitt–Savage measure is of course invariant under the evolution, and that by the linearity of (32) it commutes with the linear operator $U_\tau^{(n)}$ for all $\tau \geq 0$, it

¹¹More precisely, they are only essentially linear, for the parameters ε_0 and \mathbf{u}_0 , which also enter any of the other hierarchies whenever they describe ensembles of systems conserving mass, momentum, and energy, are all tied up with the initial conditions.

follows that at later times $\tau > 0$ the n point density of the ensemble is given by

$$f^{(n)}(\mathbf{v}_1, \dots, \mathbf{v}_n; \tau) = \langle U_\tau^{(n)} f_0^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) \rangle. \quad (45)$$

This so far simply states that, if the ensemble is initially a statistical mixture of pure states (product states), then at later times it is a statistical mixture of time-evolved initially pure states. Next we note that by inspection of (32) it follows that

$$U_\tau^{(n)} f_0^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n) = (U_\tau^{(1)} f_0)^{\otimes n}(\mathbf{v}_1, \dots, \mathbf{v}_n), \quad (46)$$

viz. pure states evolve into pure states. Every factor $f(\mathbf{v}_k; \tau) = U_\tau^{(1)} f_0(\mathbf{v}_k)$ solves (12) with $\tau = \frac{2\varepsilon_0}{3}t$, obeying the desired conservation laws. At last one can legitimately say that (12) has been derived as a full-fledged kinetic equation valid for almost every (w.r.t. $\langle \cdot \rangle$) individual member of the limiting ensemble.

6 Summary and Outlook

In summary, the diffusion equation on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ can be interpreted as the simplest “master equation” for an underlying N -body Markov process with single-particle and pair terms. The $N \rightarrow \infty$ limit for the marginal densities of solutions to the diffusion equation is well-defined and can be carried out explicitly. After invoking the Hewitt–Savage decomposition, the limit $N \rightarrow \infty$ is seen to produce solutions of the “kinetic Fokker–Planck equation” describing individual isolated systems conserving mass, momentum, and energy. The Fokker–Planck equation (9) is exactly solvable and displays correctly the qualitative behavior of a typical kinetic equation. In this sense, (9) really can be regarded as the simplest example of a kinetic equation of the “diffusive” type, in the same family as, for instance, the much more complex Landau and Balescu–Lenard–Guernsey equations.

Our work raises many new questions. 1) In particular, in Appendix Ab we have only written down the generator for the adjoint process of the underlying N -particle Markov process; hence, what is the explicit characterization of this process? 2) A derivation of a kinetic equation à la Kac is an intermediate step towards a full

validation from some deterministic (Hamiltonian) microscopic model, which is in general a very difficult program, see the rigorous derivations of kinetic equations in [Spo91, CIP94]. The substitute Markov process is usually chosen to preserve some of the essential features of the deterministic dynamics which (formally) leads to the same kinetic equation. Here we have only identified a stochastic model which leads to (9). Villani's work [Vil98] suggests that a deterministic model may exist which in the kinetic regime leads to (9). Can one indentify this model? 3) In this paper, we conveniently assumed that the Fourier coefficients ensure convergence of the marginal density functions in $\mathfrak{L}^2 \cap \mathfrak{L}^1$ and subsequently upgraded the regularity to Schwartz functions. What are the explicit conditions on the Fourier coefficients of the initial functions on $\mathbb{M}_{\mathbf{u}_0, \mathbf{e}_0}^{3N-4}$ which ensure convergence in $\mathfrak{L}^2 \cap \mathfrak{L}^1$, in Schwartz space, in some topology for measures? 4) Since the PDEs in our finite- N Fokker–Planck hierarchy are already self-contained for each n (viz., they do not involve the usual coupling to $f^{(n+1)}$), the finite- N corrections to the limiting evolutions can be studied in great detail; hence, for instance, how do the explicit corrections to propagation of chaos look? 5) We already mentioned in a footnote that the kinetic Fokker–Planck equation can easily be generalized to situations where the system is exposed to some external driving force by adding a forcing term. Can one derive this equation from some suitable ensemble of driven systems? Under which conditions do there exist stationary non-equilibrium states, and what are their stability properties? 6) Finally, our derivation is only valid for the space-homogeneous Fokker–Planck equation without driving force term; hence, can one extend our derivation to obtain the space-inhomogeneous generalization of the kinetic Fokker–Planck equation, first without and then with driving force term? These are many interesting questions which should be answered in future works.

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Appendix

A. Two useful representations of the Laplacian on spheres

Aa. Extrinsic representation in divergence form

For the purpose of obtaining equations for the marginals by integrating (14), it is advantageous to express the Laplacian on the right-hand side in terms of the projection operator $P_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ from \mathbb{R}^{3N} to the fibers of the tangent bundle of the embedded manifold $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$. It is easy to verify [KiLa04] that

$$\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}} F^{(N)} = \nabla \cdot [P_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}} \nabla F^{(N)}] \quad (47)$$

In order to have an explicit expression for $P_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}}$ we introduce an orthogonal basis for the orthogonal complement of the tangent space to $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ at $\mathbf{V} \in \mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4} \subset \mathbb{R}^{3N}$. Clearly, such orthogonal complement is spanned by the four vectors \mathbf{V} and $\mathbf{E}_\sigma = (\mathbf{e}_\sigma, \dots, \mathbf{e}_\sigma)$, $\sigma = 1, 2, 3$, where the \mathbf{e}_σ are the standard unit vectors in \mathbb{R}^3 . The vectors \mathbf{E}_σ are orthogonal to each other but not to \mathbf{V} ; projecting away the non-orthogonal component of \mathbf{V} yields

$$\left(\mathbf{I}_{3N} - \frac{1}{N} \sum_{\sigma=1}^3 \mathbf{E}_\sigma \otimes \mathbf{E}_\sigma \right) \cdot \mathbf{V} = \mathbf{V} - \mathbf{U}. \quad (48)$$

The vectors $\{\mathbf{V} - \mathbf{U}, \mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3\}$ form the desired orthogonal basis; their magnitudes are $|\mathbf{E}_\sigma| = \sqrt{N}$ and $|\mathbf{V} - \mathbf{U}| = \sqrt{2N\varepsilon_0}$. Finally, (47) becomes

$$\Delta_{\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}} F^{(N)} = \partial_{\mathbf{V}} \cdot \left[\left(\mathbf{I}_{3N} - \frac{1}{N} \sum_{\sigma=1}^3 \mathbf{E}_\sigma \otimes \mathbf{E}_\sigma - \frac{1}{2N\varepsilon_0} (\mathbf{V} - \mathbf{U}) \otimes (\mathbf{V} - \mathbf{U}) \right) \partial_{\mathbf{V}} F^{(N)} \right] \quad (49)$$

Ab. Representation for the N -Body Markov Process

In the main part of this paper we started from the diffusion equation on the manifold $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ of N -body systems with same energy (per particle) e_0 and momentum (per particle) \mathbf{u}_0 , then took the limit $N \rightarrow \infty$, obtaining the kinetic Fokker–Planck equation (12), which rewrites into (9) in view of the conservation laws. The Laplace–Beltrami operator on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ is the generator of the adjoint semigroup of

the underlying stochastic Markov process that rules the microscopic dynamics of an individual N -body system. Here we show that this generator can be written as a sum of single particle and two-particle operators, thus characterizing the Markov process as a mixture of individual stochastic motions and stochastic binary interactions. Moreover, we show that the binary particle operators are the only ones that do not vanish in the $N \rightarrow \infty$ limit. This means that the kinetic Fokker–Planck equation can also be derived in terms of an N -body stochastic process with purely binary interactions, which is more satisfactory from a physical point of view.

Recall that in section 2 we explained that $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ can be identified with the sphere $\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$ centered at the origin of \mathbb{L}^{3N-3} (which itself is an affine linear subspace of the space of all velocities, \mathbb{R}^{3N}). Recall that $\Delta_{\mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}} = \frac{1}{2N\varepsilon_0} \Delta_{\mathbb{S}^{3N-4}}$. Note the well-known representation

$$\Delta_{\mathbb{S}^{3N-4}} = \sum_{1 \leq k < l \leq 3(N-1)} \left(w_k \partial_{w_l} - w_l \partial_{w_k} \right)^2, \quad (50)$$

where w_k is the k -th Cartesian component of $\mathbf{W} \in \mathbb{S}^{3N-4} \subset \mathbb{R}^{3(N-1)}$ (note that in section 2 we used $\mathbf{W} \in \mathbb{S}_{\sqrt{2N\varepsilon_0}}^{3N-4}$, but note furthermore that the r.h.s. of (50) is invariant under $\mathbf{W} \rightarrow \lambda \mathbf{W}$). Grouping the components of \mathbf{W} into blocks of vectors $\mathbf{w}_k \in \mathbb{R}^3$, $k = 1, \dots, N-1$, the r.h.s. of (50) can be recast as

$$\begin{aligned} \Delta_{\mathbb{S}^{3N-4}} = & \sum_{k=1}^{N-1} \sum_{\substack{l=1 \\ l \neq k}}^{N-1} \left(3\mathbf{w}_k \cdot \partial_{\mathbf{w}_k} + |\mathbf{w}_k|^2 \partial_{w_l} \cdot \partial_{w_l} - (\mathbf{w}_k \cdot \partial_{\mathbf{w}_k})(\mathbf{w}_l \cdot \partial_{\mathbf{w}_l}) \right) \\ & - \sum_{k=1}^{N-1} (\mathbf{w}_k \times \partial_{\mathbf{w}_k})^2, \end{aligned} \quad (51)$$

containing one-body terms as well as binary terms. Note however that the first term in the binary sum is effectively a sum of two-body terms in disguise, which scale with factor $N-2$ and thus survive in the limit $N \rightarrow \infty$, while the true one-body sum (second line) drops out in that limit. This implies that the kinetic Fokker–Planck equation (12) can be derived from a master equation on $\mathbb{M}_{\mathbf{u}_0, e_0}^{3N-4}$ which contains *only* the binary terms (first line) in (51). This in turn implies that (12) is the kinetic equation for an underlying system of N particles with stochastic pair interactions.

B. High-Dimension Asymptotics of Associated Legendre Functions

In (30) the associated Legendre functions of degree $s = 0, 1, 2, \dots$ and order $r = 0, \dots, s$ in q dimensions occur. They are defined on the interval $[-1, 1]$ and given by

$$\tilde{P}_s^r(t; q) = \sqrt{q}^{s+r} \frac{s!}{2^r} \Gamma\left(\frac{q-1}{2}\right) \sum_{l=0}^{\lfloor \frac{s-r}{2} \rfloor} \left(-\frac{1}{4}\right)^l \frac{(1-t^2)^{l+\frac{r}{2}} t^{s-r-2l}}{l! (s-r-2l)! \Gamma\left(l+r+\frac{q-1}{2}\right)} \quad (52)$$

which differ from the $P_s^r(t; q)$ in [Mül98] in their normalization. In our investigation, $q = 3N - p$ and $t = \frac{w}{\sqrt{2N\varepsilon_0}}$, and we are interested in the limit $N \rightarrow \infty$.

The familiar asymptotics of Euler's Gamma function gives us

$$\frac{\Gamma(x)}{\Gamma(a+x)} = x^{-a} + O\left(x^{-(a+1)}\right). \quad (53)$$

for $x \gg 1$. Applying this asymptotics with $2x = q - 1 = 3N - p - 1$ and $a = l + r$ to (52), we find that given $p \in \mathbb{N}$ and $w \in \mathbb{R}$ (which implies $N > \max\{p/3, w^2/(2\varepsilon_0)\}$), when $N \gg 1$ we have

$$\begin{aligned} \tilde{P}_s^r\left(\frac{w}{\sqrt{2N\varepsilon_0}}; 3N-p\right) &= \sqrt{2}^{r-s} \sum_{l=0}^{\lfloor \frac{s-r}{2} \rfloor} (-1)^l \frac{s!}{l! (s-r-2l)!} \left(\sqrt{\frac{3}{\varepsilon_0}} w\right)^{s-r-2l} \\ &\quad + O\left(\frac{1}{\sqrt{N}}\right). \end{aligned} \quad (54)$$

By comparing with the formula for the Hermite polynomial of degree k on \mathbb{R} ,

$$H_k(x) = \sum_{l=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^{l+k} \frac{s!}{l! (k-2l)!} (2x)^{k-2l}, \quad (55)$$

we see that, given $p \in \mathbb{N}$ and $w \in \mathbb{R}$, we have

$$\tilde{P}_s^r\left(\frac{w}{\sqrt{2N\varepsilon_0}}; 3N-p\right) = \left(-\sqrt{2}\right)^{r-s} H_{s-r}\left(\sqrt{\frac{3}{4\varepsilon_0}} w\right) + O\left(\frac{1}{\sqrt{N}}\right) \quad (56)$$

when $N \gg 1$. Hence, for all fixed p we now find that pointwise for any $w \in \mathbb{R}$,

$$\lim_{N \rightarrow \infty} \tilde{P}_s^r\left(\frac{w}{\sqrt{2N\varepsilon_0}}; 3N-p\right) = \left(-\sqrt{2}\right)^{r-s} H_{s-r}\left(\sqrt{\frac{3}{4\varepsilon_0}} w\right) \quad (57)$$

where again it is understood that $N > \max\{p/3, w^2/(2\varepsilon_0)\}$ in the expression under the limit in the left-hand side. Equation (35) in the main text follows.

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